

Local Representation of N -body Coulomb Energy with Path Integrals

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We represent N -body Coulomb energy in a localized form to achieve massive parallelism. It is a well-known fact that Green's functions can be written as path integrals of field theory. Since two-body Coulomb potential is a Green's function of Poisson equations, it reduces to a path integral of free scalar field theory with three spatial dimensions. This means that N -body one also reduces to a path integral. We discretize real space with a cubic lattice and evaluate the obtained multiple integrals approximately with the Markov-chain Monte Carlo method.

Molecular dynamics (MD) is a numerical method to describe motion of N interacting particles based on Newton's classical equations of motion.¹⁾ It has been used in various fields such as structure prediction of protein,²⁾ in silico screening,³⁾ and material design. In MD of atoms, computationally the heaviest part is calculations of N -body Coulomb interaction, which explodes with operations proportional to $O(N^2)$. To propel research and development based on MD, we need to decrease turnaround time of computation by processing large amount of arithmetic operations in terms of state-of-the-art high-performance supercomputers.

There have been many efforts to decrease the number of operations to calculate N -body Coulomb interaction, such as Ewald,⁴⁾ fast multipole,⁵⁾ and Wolf⁶⁾ methods. The methods beautifully treat the non-locality associated with the long-range Coulomb interactions by dividing those into two: short and long-range regions. However, to parallelize relatively large molecules based on the methods, one has to face again the difficulty due to non-locality. There is no choice but to accept large data communications and load imbalance for massive parallelism. We cannot conduct parallel computations without exchanging the whole N or a partial sets of coordinates among computation nodes.

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One can detour around the non-locality associated with the Coulomb's long-range tails by parallelizing Markov-chain generation processes.⁷⁾ However, it is a sampling method to obtain statistical quantities such as free energy and does not simulate actual time-dependent conformations of molecules. In addition, it does not work for larger systems due to limitations on available memory size. A computation node is too small to treat a huge molecular system made of millions or more atoms. For a fundamental solution to the hard problem, we still need to find a new idea to achieve locality and parallelism.

In this letter, we rewrite a summation of N -body Coulomb energy in a local form based on path integral formulation of field theory.⁸⁾ Since everything is modeled in latticized real space, spatial decomposition is possible and gives rise to massive parallelism.

The method can take open boundary conditions. Therefore, it can treat isolated systems. Also other boundary conditions such as periodic and fixed ones are available if necessary. Any other types of boundary conditions work if those can be implemented in a field theoretic manner. The method has no conditions associated with the total charge of atoms. Therefore, it can be applied to classical gravity systems.

In this method, the number of operations necessary to calculate N -body Coulomb energy is $O(N)$. The dominant operations are fused multiply-add ones, which can be processed in parallel. As shown later, the method is suited to relatively large- N systems because it has good weak scaling property when a parallel computer is applied. As for data communication among computation nodes, one needs to perform global communication once every N -body Coulomb energy summation. This is because one needs to collect results from all the computation nodes and sum up those after all necessary calculation are done.

Let us move onto theoretical details of the method. Coulomb energy among N charged particles is a summation of two-body ones:

$$E_N = \frac{1}{4\pi} \sum_{i \neq j}^N \frac{q_i q_j}{|r_i - r_j|}, \quad (1)$$

where r_i and q_i represent a vector in three-dimensional real space R^3 and an electric charge of the i -th particle, respectively. In general, Greens' functions can be written as path integrals based on the method of generating functional in field theory.⁹⁾ Two-body Coulomb potential is inverse of Laplacian Δ

$$\Delta \frac{1}{|r|} = -4\pi\delta^3(r). \quad (2)$$

Therefore, we can represent it in a path-integral form:

$$\frac{1}{4\pi|r_1 - r_2|} = Z[0]^{-1} \frac{\delta}{\delta J(r_1)} \frac{\delta}{\delta J(r_2)} Z[J] \Big|_{J=0}, \quad (3)$$

where

$$Z[J] = \int \mathcal{D}\phi e^{-H[J]}, \quad (4)$$

and

$$H[J] = \int dr^3 \left(-\frac{1}{2} \phi(r) \Delta \phi(r) - J(r) \phi(r) \right). \quad (5)$$

$\mathcal{D}\phi$ is Feynman's path integral measure

$$\mathcal{D}\phi \propto \prod_{r \in R^3} d\phi(r). \quad (6)$$

In Eq. (4), we can integrate out the functional variable $\phi(r)$ because the integrand is Gaussian

$$Z[J] = Z[0] \exp \left[\frac{1}{2} \int dr_1^3 dr_2^3 J(r_1) \frac{1}{4\pi|r_1 - r_2|} J(r_2) \right], \quad (7)$$

which gives Eq. (3). Then, we have

$$\frac{1}{4\pi|r_1 - r_2|} = \frac{\int \mathcal{D}\phi \phi(r_1) \phi(r_2) e^{-H[0]}}{\int \mathcal{D}\phi e^{-H[0]}}. \quad (8)$$

This is a building block of our new method.

We would like to evaluate the right hand side of Eq. (8) numerically. For this purpose, we discretize three-dimensional space R^3 with a cubic lattice a^3 , where a is a spacing between two lattice sites.¹⁰⁾ Hereafter, we omit lattice spacing a for brevity. In the latticized real space L^3 , where $R = aL$, the counter part of Eq. (8) is given by

$$\frac{1}{4\pi|m - n|} \approx \frac{\int \mathcal{D}_L \phi \phi_m \phi_n e^{-H_L}}{\int \mathcal{D}_L \phi e^{-H_L}}, \quad (9)$$

where

$$H_L = \frac{1}{2} \sum_{\langle m, n \rangle} (\phi_m - \phi_n)^2, \quad \mathcal{D}_L \phi \propto \prod_{n \in L^3} d\phi_n. \quad (10)$$

We have replaced the derivative with the first-order difference. The lowercase letter m represents a position (m_x, m_y, m_z) in the lattice L^3 , where $r_x = m_x a$ and so on. The brackets $\langle m, n \rangle$ represents the set of all nearest-neighbor pairs of lattice sites.

For two-body Coulomb energy in Eq. (9), it is much easier to evaluate the left hand side than right. However, for N -body Coulomb energy with relatively large N , the path-integral

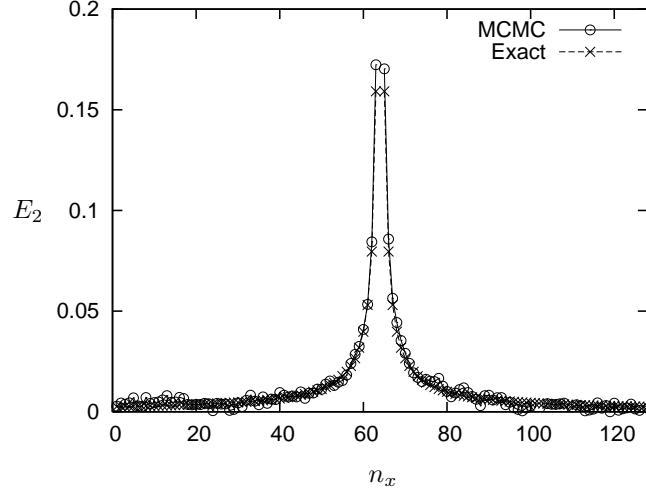


Fig. 1. The two-body Coulomb energy E_2 is compared between MCMC (circles with solid line) and the exact (crosses with dashed line) results on a lattice $L = 128$. E_2 is plotted as a function of n_x with $m_x = L/2$, $m_y = n_y = L/2$, and $m_z = n_z = L/2$ fixed. MCMC calculations have been done with the sample number $M = 10^4$.

form in the right hand side may be useful:

$$E_N \approx \frac{\int \mathcal{D}_L \phi \left[\left(\sum_{i=1}^N q_i \phi_{n_i} \right)^2 - \sum_{i=1}^N (q_i \phi_{n_i})^2 \right] e^{-H_L}}{\int \mathcal{D}_L \phi e^{-H_L}}. \quad (11)$$

We are going to evaluate the multiple integral in the right hand side with Markov chain Monte Carlo (MCMC) method. Concretely, we use the heatbath algorithm,¹¹⁾ which may be more efficient than Metropolis¹²⁾ because acceptance-rejection process is not necessary and therefore the acceptance ratio is unity. In the heatbath algorithm, a new configuration C' is generated independent of an old one C so that probability distribution P satisfies the following relation.

$$P(C \rightarrow C') \propto e^{-H_L(C')}, \quad (12)$$

which is a sufficient condition of the detailed balance. According to this, a lattice variable ϕ_n is updated with

$$r = \frac{\int_{-\infty}^{\phi_n} d\varphi e^{-\frac{1}{2} \sum_m (\varphi - \phi_m)^2}}{\int_{-\infty}^{\infty} d\varphi e^{-\frac{1}{2} \sum_m (\varphi - \phi_m)^2}}, \quad (13)$$

where r is a uniform random number $0 \leq r \leq 1$. By inverting Eq. (13), we have

$$\phi_n = -\frac{1}{\sqrt{3}}\text{erfc}^{-1}(2r) + \frac{1}{6} \sum_m \phi_m, \quad (14)$$

where the summation m is taken for all the nearest-neighbor sites of n . One can generate a new configuration C' by substituting a uniform random number r to Eq. (14). (One has to modify Eq. (14) slightly at the boundary when open boundary conditions are imposed because there is no lattice sites outside the lattice.) All the lattice variables are updated sequentially in terms of Eq. (14). Once a Monte-Carlo sample set $\{\phi_n^{(j)} : j = 1, 2, \dots, M\}$ is obtained, Eq. (11) can be approximated as

$$E_N \approx \frac{1}{M} \sum_{j=1}^M \left[\left(\sum_{i=1}^N q_i \phi_{n_i}^{(j)} \right)^2 - \sum_{i=1}^N (q_i \phi_{n_i}^{(j)})^2 \right], \quad (15)$$

where M indicates the number of Monte-Carlo samples. The number of arithmetic operations necessary to evaluate the right hand side of Eq. (15) is $O(N)$ for a fixed M . As N goes large with M fixed, there is a some point where Eq. (11) is more advantageous than (1) because direct evaluation of the latter requires operations of $O(N^2)$. One can adjust M to control statistical errors according to available computing resources. In addition, the right hand side of Eq. (15) has massive parallelism because each term contained in the summations can be evaluated independently without any information related to other particles.

In order for the method to be practical, it needs to reproduce two-body Coulomb energy accurately as much as possible because it is a building block of N -body one. Let us compare two-body Coulomb energy between MCMC and exact results, which are calculated by making use of Eqs. (15) and (1), respectively. We set $N = 2$ and $q_i = 1$ and choose open boundary conditions. We put the first particle at the center of a latticized real space, where a lattice site m takes values of $m_x = L/2$, $m_y = L/2$, and $m_z = L/2$. Then we move the second particle along a straight line $n_y = L/2$ and $n_z = L/2$ and measure energy between two. Figure 1 plots two-body Coulomb energy as a function of n_x for $L = 128$. MCMC and exact results are plotted with open circles and crosses, respectively. As for MCMC, the number of samples is $M = 10^4$. Samples are collected controlling correlations among configurations as usual. Actually, we take one sample every 1000 sweeps of L^3 lattice sites with Eq. (14). We can say that the obtained MCMC statistical average with $M = 10^4$ is good approximation to the exact one when the lattice size is $L = 128$.

In order to check accuracy of the method in many-body calculations, we measure errors

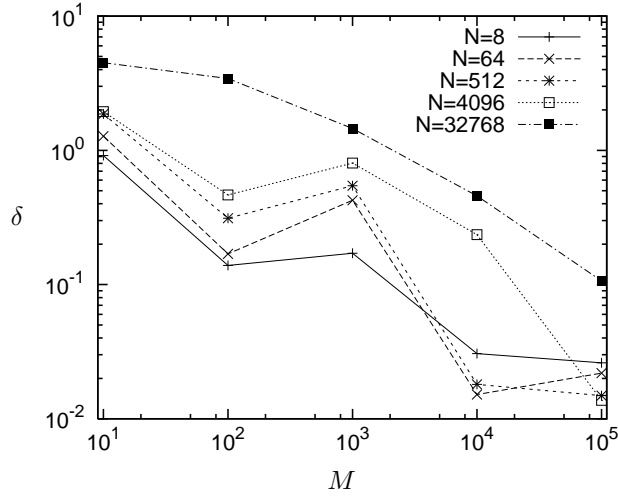


Fig. 2. The difference δ between MCMC and the exact results divided by the exact is plotted as a function of the number of MCMC samples M for various atom numbers $N = 8, 64, 512, 4096$ and 32768 on a lattice $L = 128$ with open boundary conditions.

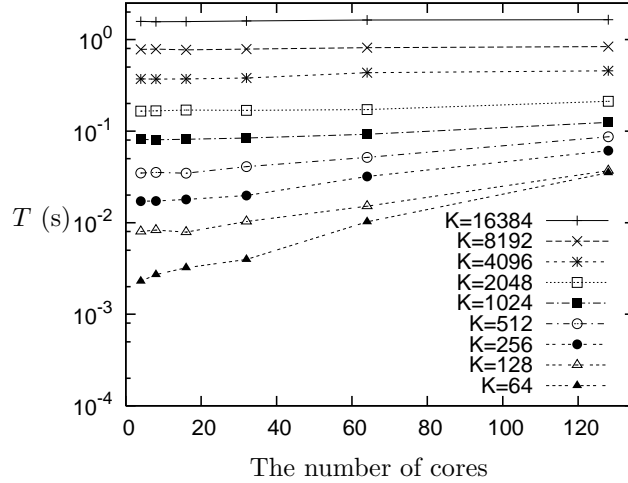


Fig. 3. Weak-scaling property of the method is shown. Elapsed time T is plotted using generated $M = 10^4$ samples as a function of the number of cores for various unit problem size $K = 64, 128, 256, 512, 1024, 2048, 4096, 8192$ and 16384 . For larger K , the plotted lines are almost flat. For smaller K , slightly increase due to use of the collective communication `mpi_reduce`.

associated with N -body Coulomb energy. Let us consider the following quantity:

$$\delta \equiv \frac{|(\text{MCMC}) - (\text{Exact})|}{|(\text{Exact})|}, \quad (16)$$

which is the difference between MCMC and exact results of N -body Coulomb energy divided by the exact. In Fig. 2, Eq. (16) is plotted as a function of the number of Monte Carlo samples

M for various numbers of particles $N = 2^3, 4^3, 8^3, 16^3$, and 32^3 on the lattice $L = 128$ with open boundary conditions. We choose all charges are $q_i = 1$ as before to show that the method works also in general cases such as gravity systems. For simplicity, we put N charged particles separately on lattice sites in a region $L/2 - N^{1/3}/2 + 1 \leq n_i \leq L/2 + N^{1/3}/2$ for $i = x, y, z$, which forms a cube. Errors associated with N -body Coulomb energy decreases as M increases, which is consistent with a well-known fact that errors associated with Monte-Carlo sampling are proportional to $1/\sqrt{M}$. We admit that the open boundary conditions affect accuracy associated with larger systems such as $N = 4096$ and 32768 . This means that, in many-body calculations with large N , we need to take a sufficiently large L to produce good approximate results avoiding boundary effects.

The most remarkable feature of the proposed method is scalability for large N in parallel computation. In order to demonstrate it, we parallelize calculations of Eq. (15) and check their weak-scaling property. We consider a rectangular parallelepiped with K lattice sites that is processed by one computation core. We put a particle on every lattice site and fix the number of lattice sites (i.e. particles). We call K the unit problem size. Therefore, the total number of particles is a product of the unit problems size K and the number of computation cores. When all the calculations are done, the results are collected from all the computation nodes and summed up to calculate Eq. (15) in terms of the MPI collective communication function `mpi_reduce`.¹³⁾ Figure 3 shows weak-scaling property of the method, where elapsed time T is plotted using generated $M = 10^4$ samples as a function of the number of cores for various unit problem size K . That is, the number of cores is changed with the unit problem size K fixed. Ideally, plotted lines should be flat because the number of operations processed by each core is identical and there is no data communication among cores. For larger K , we can say that the actual weak-scaling performance is very close to the ideal. The method can treat very large systems composed of millions or more particles with almost ideal parallel performance. On the other hand, for smaller K , we see that the plotted lines are slightly increasing because of the use of the collective communication in actual implementation of the method. This means that weak-scaling property of the method depends on the performance of the collective communication especially when K is small.

We have carried the numerical calculations on a PC cluster with Intel Xeon X5460 (3.16 GHz) processors and Infiniband inter-node connections. We have generated executable binary codes with Intel Fortran compilers.

It costs a lot to generate MCMC sample set $\{\phi_n^{(j)}\}$ because the number of necessary operations is proportional to ML^3 . To use larger L for accuracy, one needs longer CPU time

and larger storage to generate and store MCMC samples, respectively. However, a sample set can be reused once generated appropriately because it depends only on lattice size L but not positions of charged particles n_i .

To decrease errors associated with the rapidly increasing core part of the two-body Coulomb potential, one could calculate close particles directly. It does not require large data communications to do that if most of close particles are contained in the same or neighbor computation nodes.

Although we have put particles on lattice sites just for simplicity, that is not necessary. To put particles arbitrarily, one can model coordinate values of every particle in terms of the nearest eight lattice sites in three-dimensional lattice space, for example. Also one can evaluate forces among particles with interpolation in a similar way.

In this letter, we have chosen $q_i = 1$ for all the particles. Of course one can produce many-body energy with arbitrary charges in the same accuracy as the two-body energy. Errors of many-body energy comes from two-body one because N -body one is a superposition of two-body. It is important to take larger L for higher accuracy.

The proposed parallelization algorithm is quite simple because it is just a combination of fused multiple-add operations and reduction communications. It does not require any other expensive operations such as division. We can maximize the performance of the method if we have computers customized for processing those operations and communications.

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